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The model of singlet-correlated bands for temperature and doping dependences of Cu(2) Knight shift in bilayered cuprates

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Abstract

Using the model of the singlet-correlated band, the temperature and doping dependences of the planar Cu Knight shift in $YBa_2Cu_3O_7$ and $YBa_2Cu_4O_8$, at $T > T_c$, have been calculated. The spin susceptibility has been deduced by means of a Hubbard-like theory in the fast fluctuating regime. The effect of strong correlation shows up as an additional correction to the Pauli susceptibility with a strong dependence on the doping level.

Keywords: Singlet-correlated band; Spin susceptibility; Bilayered cuprates; Cuprates; Knight shift

Recently, we have shown [1, 2] that the model of the singlet-correlated bands, coupled by tunneling, allows to explain photoemission data [3, 4] for $YBa_2Cu_3O_7$ and $YBa_2Cu_4O_8$. The bonding singlet band, near the Fermi level, can be half-filled by only about 0.25 extra holes per one copper site. We now present an additional test of that model by employing NMR data [5]. Preliminary discussions using a simplified picture were given in [6].

In our calculation, we start from a Hamiltonian $H = H^a + H^b + H_{tun}$, where the superscripts a and b to the two single layers of a CuO_2 bilayer. The Hubbard-like Hamiltonian, H^a, is written as follows:

$$H^a = \sum \varepsilon_d^a \Psi_{ai}^{\sigma,\sigma} + \sum E_{pd}^a \Psi_{ai}^{pd,pd} + \sum t_{aij}^{(1)} \Psi_{ai}^{pd,\sigma} \Psi_{aj}^{\sigma,pd} + \sum t_{aij}^{(2)} \Psi_{ai}^{\sigma,0} \Psi_{aj}^{0,\sigma} + \sum t_{aij}^{(12)} (-1)^{1/2-\sigma} (\Psi_{ai}^{\sigma,0} \Psi_{aj}^{\bar{\sigma},pd} + \Psi_{ai}^{pd,\bar{\sigma}} \Psi_{aj}^{0,\sigma}) - \tfrac{1}{2} \sum J_{ij}^a [\tfrac{1}{2} - 2(\boldsymbol{S}_i \boldsymbol{S}_j)] - \sum F_i^a (\boldsymbol{S}_{i+1} + \boldsymbol{S}_{i+2} + \boldsymbol{S}_{i+3} + \boldsymbol{S}_{i+4})^2 \Psi_{ai}^{pd,pd}. \quad (1)$$

Here, $\Psi_{ai}^{\sigma,\sigma}$ and $\Psi_{ai}^{pd,\sigma}$ are Hubbard-like operators, $\boldsymbol{S}$ are spin operators, and $t_{aij}^{(1)}$ and $t_{aij}^{(2)}$ are hopping integrals between Cu sites i and j of layer a where (1) and (2) denote the singlet and the Cu band, respectively, and $t_{aij}^{(12)}$ is a hybridization parameter. Using Wannier wave functions [2], we estimated the relative values of t_{a1}, t_{a2}, and t_{a3}, where the digit denotes first, second, and third nearest neighbors, respectively. The absolute values, after being corrected in accordance with photoemission data (see Ref. [4] and references therein), are (all in meV): $t_1^{(1)} = 72$, $t_1^{(2)} = 62$, $t_1^{(12)} = -68$, $t_2^{(1)} = -1$, $t_2^{(2)} = 3$, $t_2^{(12)} = -1$, $t_3^{(1)} = 13$, $t_3^{(2)} = 9$, and $t_3^{(12)} = -11$.

In (1), ε_d^a and E_{pd}^a are the site energies of Cu holes and Cu–O singlets, respectively. It is clear that the singlet band must be located below the empty Cu hole states d_{xy} and $d_{3z^2-r^2}$. We have estimated that

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